# Simulation and experimental studies of Al metal matrix composites reinforced with $Fe_3Al$ intermetallics

A thesis submitted in partial fulfillment of the

requirements for the degree of

**Master of Technology**

**In**

**Mechanical Engineering**

**By**

**Sarat chandra venumbaka**
**(Roll No-213MM2489)**


Department of Metallurgical and Materials Engineering
National Institute Of Technology,
Rourkela-769008, Odisha, India
May-2015.

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Under the guidance and supervision of

**Prof. S.N. Alam**

**and**

**Prof. N. Yedla**


Department of Metallurgical and Materials Engineering
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Rourkela-769008,Odisha,India

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**DEPARTMENT OF METALLURGICAL & MATERIALS ENGINEERING**
**NATIONAL INSTITUTE OF TECHNOLOGY, ROURKELA**

# Certificate

This is to certify that the Project Report entitled "**Simulation and experimental studies of Al metal matrix composites reinforced with $Fe_3Al$ intermetallics**", submitted by **Mr. Sarat chandra venumbaka (213mm2489)**, in partial fulfilments for the needs for the award of **Master of Technology** Degree in **Mechanical Engineering** at **National Institute of Technology, Rourkela,**is an authentic work executed by him under my direction and guidance. To the best of my awareness, the substance embodied in the report has not been submitted to any other University / Institute for the award of any Degree.

**Date:**

**Prof. S.N. Alam**

Assistant Professor
Department of Metallurgical & Materials Engineering
National Institute of Technology, Rourkela


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**Date:**

**Prof. Natraj Yedla**

Assistant Professor
Department of Metallurgical & Materials Engineering
National Institute of Technology, Rourkela

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**Sarat chandra venumbaka**

**(213mm2489)**

**Metallurgical & Materials Engineering**

**National Institute of Technology, Rourkela**

# ABSTRACT

In this thesis molecular dynamics simulation (MD) and experimental compressive deformation studies on the mechanical properties of Al metal matrix composites reinforced with different volume fractions (5%, 10%, 15% and 20%) of $Fe_3Al$ intermetallics is investigated. The studies are carried out at different strain rates ($10^{11}s^{-1}$, $10^{10}s^{-1}$, $10^{9}s^{-1}$ and $10^{8}s^{-1}$) and temperatures (10K, 50K, 100K, 200K and 300K). The Aluminium and its alloys have excellent ductility but reasonable strength makes it widely used in the field of automotive, aerospace. Nowadays Al-based composites are used due to their superior mechanical properties. The reinforcements added to MMC will improve the properties of the composite like yield strength, hardness, density and wear behavior. The reinforcements are ceramic, metallic and non-metallic used in the form of particles, fibers, and laminates. There are several studies done on the non-metallic and ceramic reinforcements. However, there are least studies done on the reinforcement such as $Fe_3Al$ on the mechanical behavior. In this study Al-$Fe_3Al$ composite is synthesized by mechanical alloying (MA). In MD simulation a box of dimension $50\times100\times50$ $Å^3$ is created with 15708 atoms. The $Fe_3Al$ particles are reinforced as spherical clusters in Al matrix all over the volume. This composite is subjected to different loading conditions and temperatures. Inter atomic forces are calculated by using the embedded atom method (EAM). With the help of Ovito software the structural changes have studied, and from the stress-strain plots the changes in mechanical properties have been observed. In Fig.1, it has been observed that with an increase in the volume fraction of reinforcement from 5% to 20% the compressive strength of the material is increasing. These results have been compared with the experimental results. It was found that the strength of the composite is increasing with reducing the temperature and adding of $Fe_3Al$ intermetallics to the Al metal matrix increases the yield strength and hardness.

Key Words: Molecular Dynamics, LAMMPS, Srain rate, MMC

# Table of Contents

# CHAPTER 1

## 1.1 Background

In recent years significant use has been made of digital computers to analyse the various aspects of molecular dynamics in solids, liquids, and gases [1]. The crystalline structure or atomic arrangement of a material is very important in determining the properties and behavior of a solid material. Aluminum is one of the most widely used metals due to its desirable physical, chemical and mechanical properties and it characterizes an important category of technological materials. Because of its high strength-to weight ratio, besides other desirable properties e.g. high corrosion resistance, desirable appearance, nonmagnetic, non-sparking, non-toxic, ease of fabrication and high thermal and electrical conductivities, aluminum and its alloys are used in a wide variety of industrial applications. These properties led also to the association of aluminum and its alloys with transportation mainly with aircraft and space vehicles, containers and packaging and electrical transmission lines, construction and building [2]. Nowadays Al-based composites are used due to their superior mechanical properties. The reinforcements are ceramic, metallic and non-metallic used in the form of particles, fibers, and laminates. The reinforcements added to MMC will improve the properties of the composite like yield strength, hardness, density and wear behavior. There are several studies done on the non-metallic and ceramic reinforcements. However, there are least studies done on the reinforcement such as $Fe_3Al$ on the mechanical behavior. Inter metallics such as $Fe_3Al$ are used as reinforcement in the present study.

Inter metallic compound is a phase formed at intermediate composition of two primary components (pure metals). The crystal structure of compound obtained is different from both primary components. Inter metallics are similar to alloys, but the bonding between the atoms is partially ionic, leading to different properties than traditional alloys. Iron aluminides are also an inter-metallic compound of pure metals iron and aluminium.

Inter-metallic alloys such as iron aluminides have been much investigated over the last few years, mostly in the USA, but also in India, japan, and some European countries, because of their excellent properties relative to other engineering alloys. The possible application as lower density alternative for stainless steels at moderate temperatures (500–600°C) and in different oxidizing or corrosive atmospheres makes it an interesting component to study.

In our study the molecular dynamics method is applied to study the mechanical properties of Al metal matrix composites reinforced with $Fe_3Al$ intermetallics. One of the main particularities of the classical molecular dynamics is a variety of model potentials of inter atomic interaction, specifically when metal systems are under discussion. We used the embedded atom method (EAM) based on the potential, which consists of many-body contribution to the interaction taking into account atomic density distribution. On the other hand the EAM can be easily combined with the molecular dynamics method and it is proved to give highly reliable results for a number of pure liquid metals and some alloys [3]. All strengthening techniques depend on simple principal of restricting dislocation motion, which increases the strength and hardness of the material. The strengthening mechanisms can be introduced by solid solution, precipitation hardening, strain hardening and grain size reduction. Fine grain size is often preferred for high strength. Fine clusters and thin sheets of reinforcements may be added to increase strength of the alloy [4]. Mechanical properties of Al-$Fe_3Al$ composites depend on the extent of $Fe_3Al$ reinforcement.

# CHAPTER 2

# 2 Literature review

## 2.1 Introduction

A composite is a material having two or more physically and/or chemically different phases. The composite materials have improved properties than those of each of the base components. Generally the reinforcing material is distributed randomly all over the matrix. When the base component is a metal, then the composite is called as a metal-matrix composite (MMC). In MMC's, the reinforcing component usually is in the form of whiskers, particles, continuous fibers, or short fibers. The MMC's are characterized by the properties of the reinforcement such as short fiber- reinforced MMC's, particle reinforced MMC's, and layered MMC's or continuous fiber MMC's. These composites are differentiated by the aspect ratio (length/diameter) and diameter of the reinforcement. The aspect ratio is of great importance, because the rate of load transfer to the reinforcement from the matrix is directly proportional to the aspect ratio of the fiber. Thus, layered fibers provide highest rate of energy transfer, because of the very large aspect ratio, which results in strengthening of the composite along the direction of fiber. Metal composites have found application in many daily life applications. These materials are manufactured in situ from the conventional processing and production of metals. These materials show unlimited possibilities for modern material development. The properties of the material can be improved dependent on the requirements of the application. The flexibility of mixing various material systems (metal - ceramic - non-metal) gives the possibility for different variations.

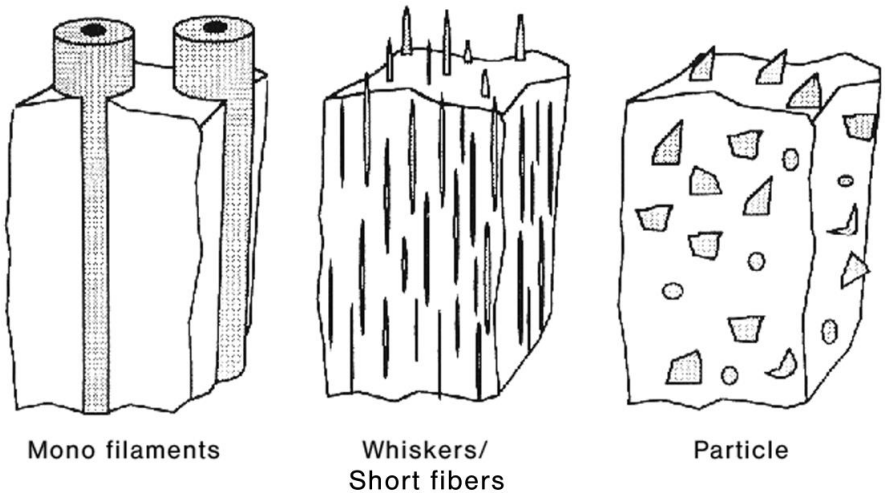



Fig.2.1 Schematic presentation of the various shapes of MMC materials [8].

## 2.2 Processing of Metal Matrix Composites

Metal matrix composite materials can be created by a wide range of procedures. The center of the choice of suitable procedure designing is the fancied kind, amount and dispersion of the reinforcement (particles and fibers), the matrix alloy and the application. By adjusting the assembling technique, the handling and the finishing and by the type of the reinforcement it is conceivable to acquire diverse trademark profiles, despite the fact that the same arrangement and measures of the parts are included. These can be produced by different techniques. Some of them are listed below.

- Casting or liquid infiltration.
- Squeeze casting or pressure infiltration.
- Diffusion bonding.
- Deformation processing.
- Powder processing.
- Sinter-forging.

### 2.2.1 Powder processing

In our present study, metal matrix composites are prepared by powder processing route. These processes are used to produce short fiber or particulate reinforced composites. Compaction and sintering are performed in this process. The matrix and reinforcement powder are first mixed to produce a uniform distribution. This blending is trailed by compaction to produce a green pellet, which is approximately 80% dense and easy to handle. This green body is degassed in a sealed container in order to remove any moisture absorbed from the surroundings. Then the pellet is hot pressed to prepare a dense composite and molded into required shape.

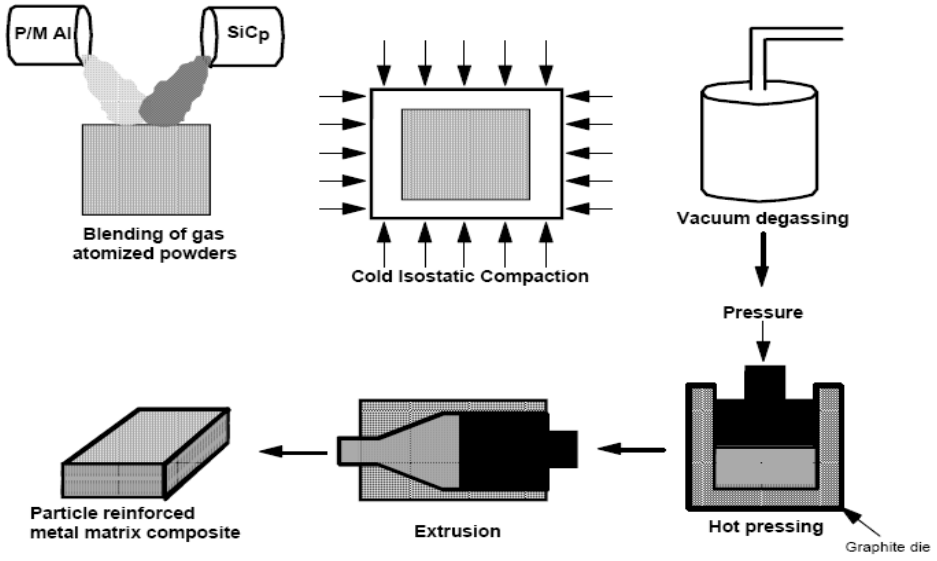



Fig. 2.2 Powder processing for fabricating short fiber reinforced MMCs [21].

## 2.3 Properties of MMC's

### 2.3.1 Young's modulus

Fiber-reinforced MMC's shows an increase in the longitudinal Young's modulus as a function of particle volume. Whereas the modulus increase in a direction perpendicular to the fibers is much lower.[22] Reinforcement volume also increases the modulus of the composite. Figure 2.3 shows change in Young's modulus in aluminum MMC with volume fraction of SiC particles. Note that due to the distribution of the particles along the extrusion axis, the modulus along the longitudinal orientation is higher than the perpendicular orientation. So reinforcement efficiency will be improved by using continuous fiber over particle reinforcement. Metal-matrix composites such as SiC particle-reinforced Al can offer an increase of 50-100% in Young's modulus over that of pure Al, i.e., approximately equivalent to that of titanium but about 33% less dense. The stiffness distribution of particle reinforced composites is homogeneous when compared with fiber-reinforced composites.

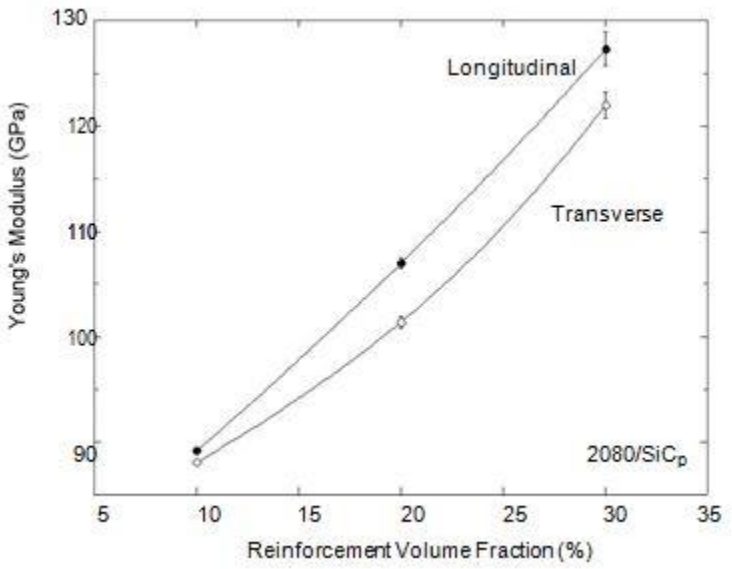



Fig. 2.3 The change in Young's modulus of aluminium composite with reinforcement volume fraction [22].

### 2.3.2 Toughness

Toughness can be defined as the resistance to crack propagation or the measure of energy absorbed in the process of fracture.[23] The toughness of the metallic composite depends on the matrix composition, reinforcement size, type, and orientation. For a fixed volume fraction of the fiber, the larger the fiber diameter, the tougher will be the composite.

### 2.3.3 Thermal stress

In general most metallic matrices have a coefficient of thermal expansion higher than that of ceramic reinforcements (whiskers, fibers, or particles). This results in generation of thermal stresses in both the components when subjected to a temperature change. Figure 2.4 shows a atomic simulation of stresses in Al matrix composite reinforced with SiC particles due to temperature changes. Here thermal residual stresses are developed in the Al and SiC, and they are worsened in regions of particle clustering.

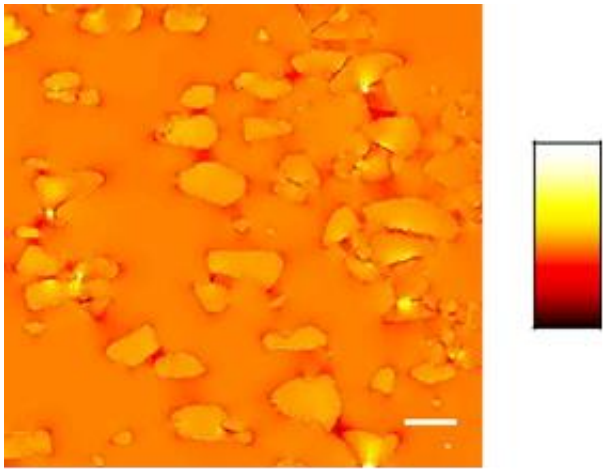


Fig. 2.4 Microstructure based simulation of an Al matrix composite reinforced with SiC particles showing thermal residual stresses [24].

### 2.3.4 Fatigue

This is the process of degradation of mechanical properties leading to failure of a component or material subjected to cyclic loading.[25] Most of the high volume practices of MMC's involve cyclic loading conditions. Processing related defects like particle clusters or intermetallic inclusions play a major role as crack initiation sites, particularly in materials processed by powder metallurgy route. Figure 2.5 shows that with increase in volume of the particles reinforced the fatigue strength of the composite is increasing.

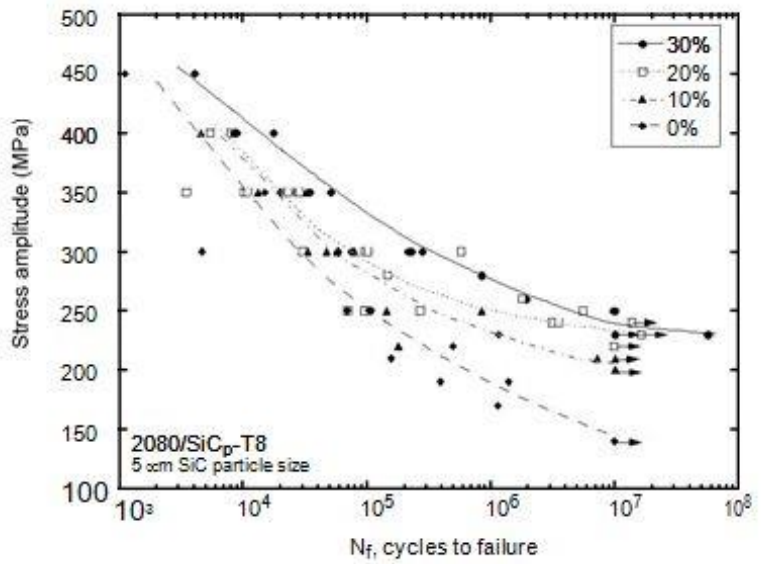



Fig. 2.5 stress amplitude Vs cycles to failure [26].

## 2.4 Advantages and properties of Aluminium

Aluminium has the highest proportion of the metals available in the Earth's crust. Due to the high availability, better strength to weight ratio and its mechanical properties, it is one of the most used non-ferrous metals in the recent past. Aluminium metal is very light with a specific weight 2.7 $g/cm^3$. The use of aluminium helps in reducing the dead weight of the vehicle, which in turn reduces energy consumption. By changing the composition of its alloys, it can be used in high strength applications also. Aluminum will generate an oxide coating which will makes it highly corrosion resistant. It is mainly useful in anti-corrosive applications where protection is required. Aluminum has a very good thermal and electrical conductivity and in relation to its weight it is more conductive than copper. So in the manufacture of power transmission lines mostly aluminium is used.

## 2.5 Iron aluminides.

Inter metallic compound is a phase formed at intermediate composition of two primary components (pure metals). The crystal structure of compound obtained is different from both primary components. Inter metallics are similar to alloys, but the bonding between the atoms is partially ionic, leading to different properties than traditional alloys. Iron aluminides are also an inter-metallic compound of pure metals iron and aluminium. The iron aluminides will have a combination of very good physical, mechanical and thermal properties. These can be used in high temp. sulfidizing oxidizing environments, resistance heating elements, automotive components, rotating parts, porous gas metal filters. They resist corrosion by the formation of an adherent surface film of $Al_2O_3$. Iron aluminide is also more ductile then stainless steel. These properties, among others, make a better material for some applications, despite its slightly higher cost.

Table 2.1 Experimental studies done on Aluminum based metal matrix composites

| Alloy/composites | Matrix | Reinforcement | Significant results | Mode of deformation | Reference |
|---|---|---|---|---|---|
| **composite** | Al | $Al_2O_3$ | Yield strength is increasing | tension | 7-8 |
| **composite** | $Fe_3Al$ | $Al_2O_3$ | Compressive yield strength is improved. | compression | 9 |
| **composite** | Al | $Si_3N_4$ | Tensile strength is improved | tension | 10 |
| **composite** | Al/Si | Aluminosilicate | UTS is improved | tension | 11 |
| **composite** | Al | $Fe_3Al$ | synthesis | | 12 |

Table 2.2 Simulation studies done on Aluminum based metal matrix composites

| Alloy/composites | Matrix | reinforcement | Significant results | Type of simulation | Reference |
|---|---|---|---|---|---|
| **Composite** | Al | Si | Effect on yield strength is found | MD | 13-14 |
| **composite** | Al | Si | Deformation mechanism | MD | 15 |

## 2.6 Gaps in the Literature

1. Several experimental studies [7-12] have been reported on the effect of reinforcement (Si3N4, Al2O3 and Aluminosilicate) on the mechanical properties of Al metal matrix composites. However, there are seldom studies reported on the influence of $Fe_3Al$ intermetallics as a reinforcement on the mechanical properties of Al-metal matrix composites.
2. Several simulation studies such as tensile compression bending have been reported on the effect of reinforcement (Si and Al2O3) on the mechanical properties of Al metal matrix composites. [13-15] However, there are seldom studies reported on the influence of $Fe_3Al$ intermetallics as a reinforcement on the mechanical properties of Al-metal matrix composites.
3. The critical volume fraction of the reinforcement, influence of temperature and strain rate on the stress-strain response is also not reported in literature.

# CHAPTER 3

# 3 COMPUTATIONAL AND EXPERIMENTAL METHOD

## 3.1 Computational method

### 3.1.1 Motivation

We perform computer simulation because of its ability to give the information of atoms as far as their structure and the delicate connections between them. This encourages us to learn something new, something that can't be created in different ways. The two principle families of simulation approaches are Monte Carlo (MC) and Molecular Dynamics (MD); also, here is an entire scope of crossover strategies which consolidate highlights from both. In this address we should focus on MD. The incontestable preference of MD over MC is that it gives a dynamical study of the framework: time-subordinate reactions to irritations, transport coefficients, deformation properties and spectra.

### 3.1.2 Molecular Dynamics (MD)

Molecular Dynamics (MD) is a computer simulation method where the time development of a set of interacting atoms and molecules of a system subsequently integrating their equations of motion. The particles and atoms of the framework are permitted to communicate for a period of time giving a perspective of their movement. The directions of the interfacing particles are dictated by numerically settling Newton's comparisons of movement where strengths between the particles and potential vitality are characterized by atomic mechanics power fields. The Newton's equation of motion can be articulated as:-

$$F_i = m_i a_i$$

$$a_i = \frac{d^2 r_i}{dt^2}$$

Where

F= force between the interacting particles

$m_i$= mass of the particle

$a_i$ = Acceleration of the particle

$r_i$= particle position

The following steps are followed while doing molecular dynamics simulation:-

- The depiction of introductory positions and velocity of each atom are done.
- The interatomic possibilities are utilized to examine the strengths between these molecules. After a little interim of time the powers are recognized, the nuclear positions and speeds changes to another state.
- The recurrence of recognizable proof of positions and velocity is completed until the end of the simulation.
- The energy remains constant due to no mass modification occurs in the system throughout the simulation.

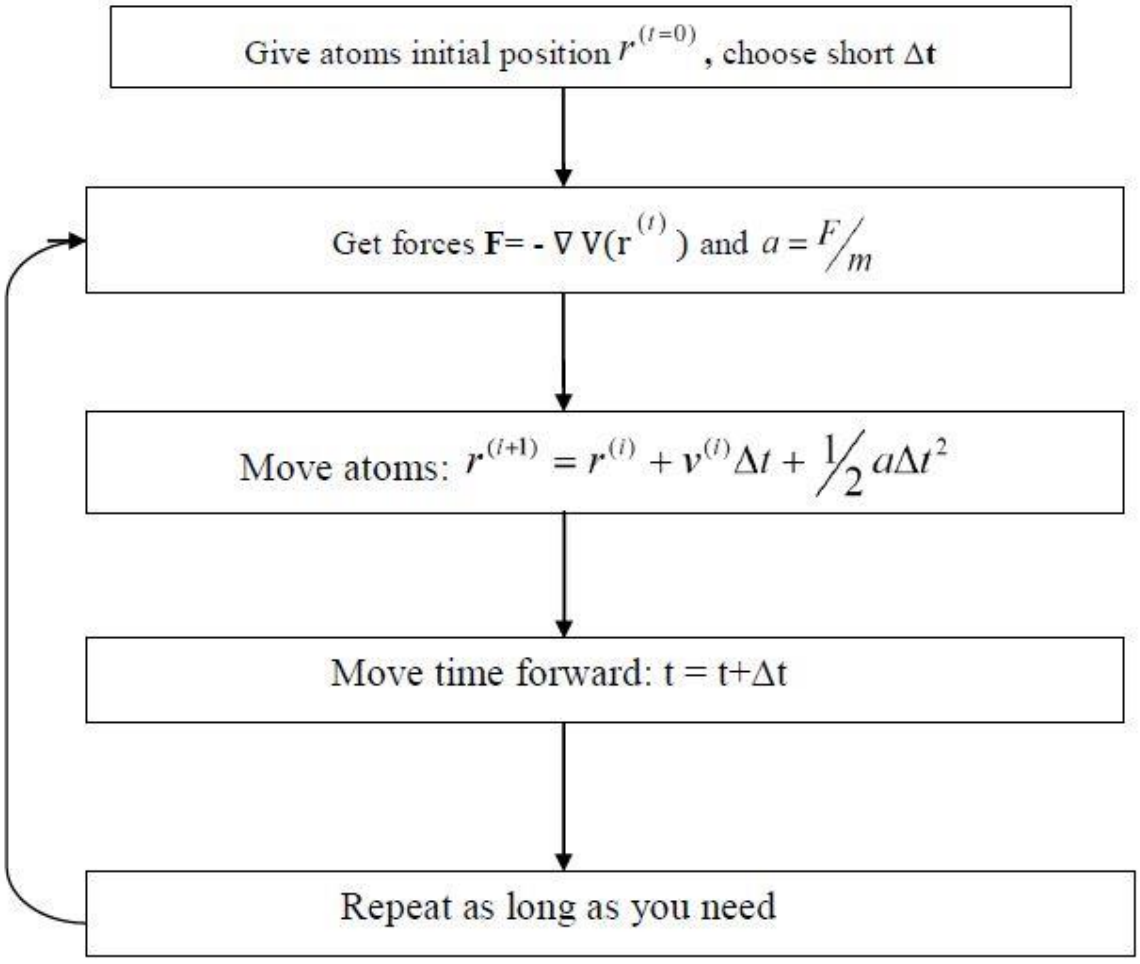



Fig. 3.1 Simulation hierarchy flowchart

### 3.1.2.1 Boundary Condition

For successively MD simulation, the decision for the Boundary Condition (BC) is extremely essential. Because of the confinements in computer productivity; Molecular Dynamic recreation can give a little gathering of molecules of the framework under analysis. For the most part there are two most vital limit conditions, one is Isolated Boundary condition and another is Periodic Boundary Condition. In Isolated Boundary Condition the molecules or particles connect with themselves however can't associate with outside particles. At the same time, in the event of Periodic Boundary Condition the particles communicate with themselves as well as associate with outside particles.

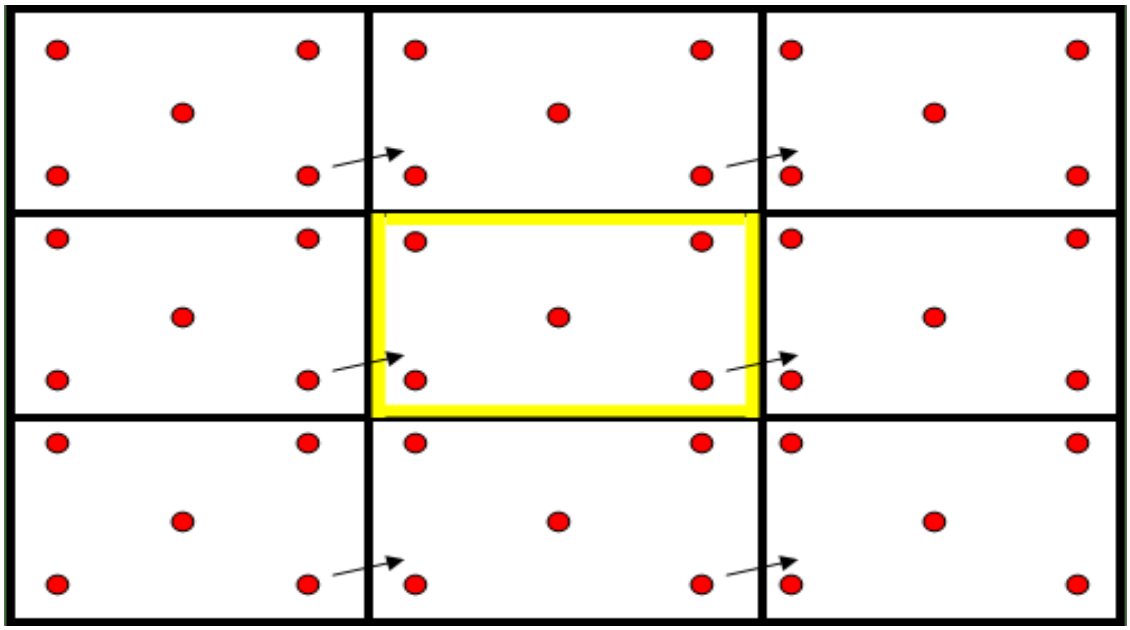


Fig. 3.2 2-D representation of Boundary Conditions

### 3.1.2.2 Interatomic Potentials

Interatomic potential is characterized as the cooperation between pair of molecules or gathering of particles in a fluid stage. On the off chance that pairing happens between the atoms, potential must be having both the natures i.e. attractive and repulsive. It is the important part of MD simulation. In MD simulation we revise millions of particles and there are different type of computation is required like- transport calculation (diffusion, thermal conductivity, viscosity)

mechanical quantities (elastic constant, plastic yield), and also the modelling of compound phenomena (shear band localization). Output results bank on the eminence of interatomic potential. On the off chance that basic possibilities are utilized, there is less accurateness while for extensive simulation, more complex potential give a superior result. Such a large number of quantities of possibilities are utilized as a part of simulation procedure. There are some important potential are described underneath:

### 3.1.2.2.1 Empirical Potential

It is the mix of intra-atomic and between sub-atomic commitments. An intra-atomic potential vitality capacity contains the short-range or reinforced bit of the potential while between sub-atomic potential vitality capacities contains the long range or non-fortified connections. Numerical manifestation of observational potential is given beneath:

$$V = V_{\text{Short-range}} + V_{\text{long-range}}$$

### 3.1.2.2.2 Pair Wise Potentials

In Molecular Dynamics, various type of pair potential available to depict numerous atom/molecule interactions, for instance Born-Lande potential, which is frequently used to define ion lattice. The Morse potential is an experimental potential that clarifies the extending of a substance bond with its unbalanced design which will be discovered to be troublesome to pack a bond as contrasted with pulling a bond separated.

### 3.1.2.2.3 Multiple-body Potentials

In multiple-body potentials, the potential energy incorporates the impacts of three or more particles associating with every other. In pair-wise potentials, worldwide interfaces in the system also occur, but they happen only through pairwise terms. But in multiple-body potentials, the potential energy can't be found by a whole over sets of atoms, as these communications will be ascertained unequivocally as a mix of higher-order terms.

### 3.1.2.2.4 Embedded Atom Method

EAM method plays a vital role in molecular dynamics simulation. In EAM, total energy is the addition of separation between the atoms & its neighbour atoms. The EAM method will be figured sober-minded by fitting to the sublimation energy, balance cross section consistent, elastic constants and vacancy creation energies of the pure metals and the heats of the solutions of the binary alloys. If there are N numbers of atoms in the system, then the total energy of the system can be expressed as below:-

$$E_{total} = \sum_i F_i(\rho_{h,i}) + \frac{1}{2}\sum_{\substack{i,j \\ i \neq j}} \emptyset_{ij}(R_{ij})$$

### 3.1.2.3 Ensembles

Time midpoints are journalist to the outfit midpoints will be the major thought for assessing the simulation results. Mostly, MD simulation is carried out under some vital equilibrium ensembles. Some commonly used ensembles are itemized below:-

**Micro-canonical or NVE ensemble:**

The expansion of NVE is N (no. of atoms/molecules), V (volume) and E (energy). It is considered as total energy remains constant throughout the simulation.

**Canonical or NVT ensemble:**

In NVT, number of particles(N), Volume (V) and Temperature (T) are conserved. Here temperature is constant throughout the simulation for which it is also called as constant temperature molecular dynamics. In NVT, because of thermostat the endothermic & exothermic processes can be exchanged.

**Isothermal-Isobaric or NPT ensemble:**

In NPT, number of particles (N), Pressure (P) and Temperature (T) are conserved throughout the simulation.

**Isenthalpic-Isobaric or NPH ensemble:**

In NPH, number of particles (N), Pressure (P) and Enthalpy (H) remains constant throughout the simulation.

## 3.1.2.4 Integration

In MD simulation, the forces should be incorporated for the movement of atoms. Because of million numbers of atoms participate in the simulation it is very tiresome and difficult to analyse a system. Therefore, a system is functional to a numerical integration method. Hence numerical integration method consists of several methods such as-Verlet algorithm, Velocity-Verlet algorithm, Leap-frog algorithm and Beeman's algorithm. Among them Verlet algorithm is essentially used in molecular dynamics simulation.

**Verlet Algorithm:**

In molecular dynamics, the most frequently used time integration algorithm is undoubtedly called Verlet algorithm. The fundamental thought is to compose two third-arrange Taylor extensions for positions ***r(t),*** one frontward and one retrograde in time. The third order extents will be velocities ***v(t)***, acceleration ***a(t)*** and the third order derivative of positions ***b(t).***

$$r(t-\Delta t) = r(t) - v(t)\Delta t + \frac{1}{2}a(t)\Delta t^2 - \frac{1}{6}b(t)\Delta t^3 + O(\Delta t^4)$$

$$r(t+\Delta t) = r(t) + v(t)\Delta t + \frac{1}{2}a(t)\Delta t^2 + \frac{1}{6}b(t)\Delta t^3 + O(\Delta t^4)$$

By adding above expressions following expression can be derived:

$$r(t+\Delta t) = 2r(t) - r(t-\Delta t) + a(t)\Delta t^2 + O(\Delta t^4)$$

This is the basic form of Verlet Algorithm.

### 3.1.2.5 Application of Molecular Dynamics simulation

- ✓ Used to study the impact of neutrons and particle light on strong surfaces.
- ✓ It has wide applications in materials segments too where tests in regards to any issue are extremely hard to do in research centre conditions.
- ✓ It is basically utilized for simulation of bio-sub-atomic frameworks like protein synthesis and classification.
- ✓ It is additionally used to study different properties of metals, non-metals and compounds like high temperature behaviour, fatigue properties, deformation behaviour and tensile properties.

## 3.2 LAMMPS

LAMMPS (Large-Scale Atomic Molecular Massively Parallel Simulator) is a Molecular Dynamics program developed by Sandia National Laboratories. This is the simple code to perform material simulation. LAMMPS can be used as a parallel molecule test system at the nuclear, or continuum scale. It is utilized to run in single or parallel processors using message-passing parallelism (MPI).

LAMMPS is completed by giving the input script command. Each order drives LAMMPS to make some operation and it stops when the data script ends.

The structure of a input script in LAMMPS is:

1. Initialization.
2. Atom and Lattice description.
3. Force fields.
4. Settings.
5. Run a simulation.

**The following commands describe the input file of the program:**

**Initialization:**

The metal units are going to be used in the simulation i.e. metal units are: distance ( Å), energy( eV), time( picoseconds), temperature(K), velocity( Å/ps), pressure(bar).

Units metal

Echo both

The boundary conditions that are used in LAMMPS are:

P P P

S P S

P F P

Where, "P" represents periodic, "F" represents non-periodic & fixed and "S" represents non-periodic &shrink-wrapped.

Box dimensions used in LAMMPS:

Dimension 3 or 2

**Atom & Lattice description:**

Atom_style atomic
region box block 0 50 0 50 0 50 units box
create_box 3 box

**Definition of the type of lattice:**

```
Lattice          FCC 4.05
```

**Definition the region that is going to be studied**:

```
region           Al block 0 50 0 100  0 50 units box
create_atoms      1 region Al units box
region           2 sphere 10 10 10 20 units box
region           2 delete

lattice          fcc 2.87
region           fe sphere 10 10 10 20 units box
create_atoms     2 region fe units box
```

**Force field:**

```
set              region fe type/fraction 3 0.25 12358
```

Choice of the interatomic potentials plays an important role throughout the simulation. The "*" represents that the potential to be applied between the atoms.

```
pair_style       eam/alloy

pair_coeff       * * FeAl.set Al Fe Al
```

**Setting:**

Energy minimization plays a vital role in LAMMPS. Higher the energy minimization higher is the stabilization among the atoms and vice-versa.

```
minimize          1.0e-3 1.0e-6 10000 100000
```

thermo 100

thermo_style custom step temp press pe ke etotal

The output of the simulation is obtained in text files called dump files. It contains the information of the atom coordinates along with the velocities dumped at the given time step.

dump a all atom 100 reinforce_feal.lammpstrj

dump_modify a scale no log heat_10^13ks-1.data
velocity all create 300 87387 rot yes dist gaussian

**Run the simulation:**

compute myRDF all rdf 50
fix 2 all ave/time 50 1 50 c_myRDF file reinforce_feal.rdf

fix b all npt temp 300 1500 0.1 iso 0.0 0.0 0.1
run 1000
unfix b

## 3.3 Experimental method and materials

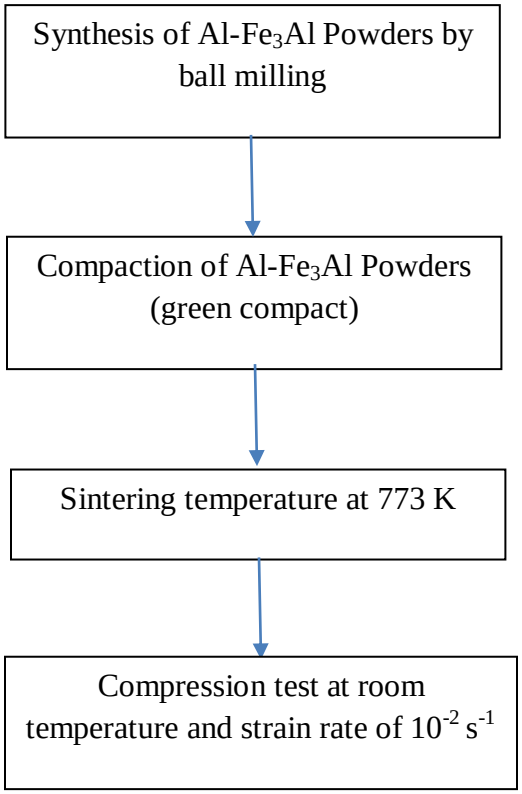



Fig. 3.3 Flow chart showing the sequence of operations

In this experimental study, the effect of 10% volume fraction of $Fe_3Al$ on Al metal matrix in compressive deformation is observed. For this purpose two samples are prepared. One of them is made of pure Al and the other is Al matrix reinforced with 10% volume fraction of $Fe_3Al$. The weights of the powders required are calculated by using the following formula.

$$v_c = v_m + v_f$$

$$v = \frac{m}{\rho}$$

Where $v_c = volume\ of\ composite$

$v_m = volume\ of\ matrix$

$v_f = volume\ of\ fiber$

$\rho = density\ of\ the\ powder$

$m = mass\ of\ the\ powder$

By using the above formula the weight of the Al and $Fe_3Al$ powders required to prepare the sample of weight 3g is found. From the data obtained 2.35g of Al and 0.65g of $Fe_3Al$ powders are used in the preparation of sample. These powders are mixed homogeneously and are compacted by applying a load of 4 ton using a die of 25mm. Cold compaction machine was used in this process.

Fig. 3.4 Hydraulic press used for compaction

Then a green pellet is obtained, and this pellet is sintered in an inert atmosphere in a furnace to remove the moisture present in the material. The sintering process is carried out at 773K for two hours and holding for one hour in argon atmosphere.

Fig. 3.5 The electric furnace used for sintering

The specimens obtained after the sintering process are polished with the help of emery paper to obtain a flat surface. Then the specimens are placed in universal testing machine and a compressive load is applied at a strain rate of $10^{-2}$ $s^{-1}$.the compressive test is performed by using the Instron universal tensile machine. After the compression test has been completed, the load vs displacement curve is generated and the results are analyzed.

## 3.4 Objectives

a) To study the effect of $Fe_3Al$ reinforcement on the mechanical properties of Aluminium metal matrix composites.

b) To perform molecular dynamics simulations for identifying the deformation mechanism and the role of $Fe_3Al$ on the nature of the stress-strain behavior.

c) To investigate the effect of volume fraction (5 vol. %, 10 vol. % 15 vol. % and 20 vol. %) of $Fe_3Al$ intermetallic on the nature of the stress-strain behavior in Al-$Fe_3Al$ metal matrix composites.

d) To study the effect of strain rate ($10^8$ $s^{-1}$, $10^9$ $s^{-1}$, $10^{10}$ $s^{-1}$ and $10^{11}$ $s^{-1}$) on the compressive deformation behavior Al-$Fe_3Al$ metal matrix composites.

e) To study the effect of temperature (300K, 200K, 100K, 50K and 10K) on the compressive deformation behavior of Al-$Fe_3Al$ metal matrix composites.

# CHAPTER 4

# 4. RESULTS AND DISCUSSIONS

## 4.1 Experimental studies

In order to find out the effect of $Fe_3Al$ reinforcement on the Al metal matrix, a compressive deformation study is carried out. The Al MMC with 10% volume reinforced with $Fe_3Al$ particles is compressed with the help of a universal testing machine, and the results are compared with the results of pure Al matrix tested under the same loading conditions. Fig.4.1 shows the variation of strength of the matrix with the $Fe_3Al$ volume. The Young's modulus of the matrix is increasing from 40.62 GPa to 42.12 GPa with addition of 10% volume fraction of $Fe_3Al$ reinforcement. These results are validated by using molecular dynamic study. The critical volume of the reinforcement to be used to improve the strength is found out by varying the volume percentage of $Fe_3Al$ particles.

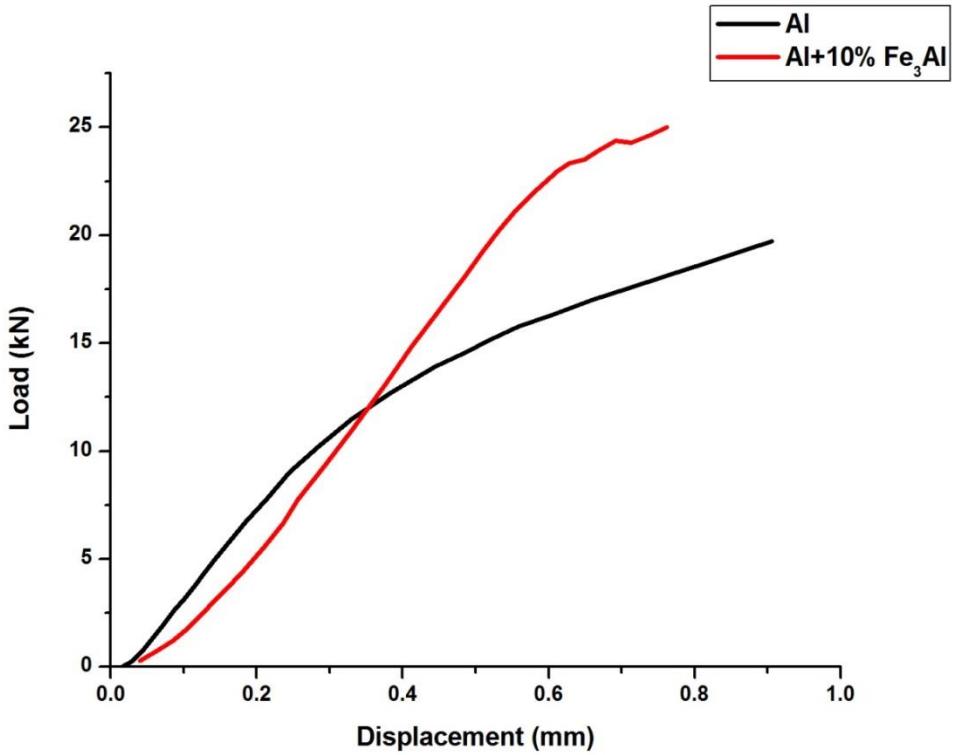



Fig.4.1 Load vs displacement curve in compressive deformation

## 4.2 Creation of Al matrix composite reinforced with $Fe_3Al$ intermetallics by MD

An Al metal matrix composite is created by reinforcing $Fe_3Al$ particles in the form of clusters all over the volume. The mechanical properties of Al metal matrix composites reinforced with different volume fractions (5%, 10%, 15% and 20%) of $Fe_3Al$ intermetallics is investigated. The compressive studies are carried out at different strain rates ($10^{11}s^{-1}$, $10^{10}s^{-1}$, $10^{9}s^{-1}$ and $10^{8}s^{-1}$) and temperatures (10K, 50K, 100K, 200K and 300K). After the compressive test, mechanical properties such as ultimate tensile strength, Young's modulus and yield strength has been evaluated.

- This program is for observing the compressive behavior of Al MMC reinforced with 10 volume percentage of $Fe_3Al$ for 3D system ($10^{10}s^{-1}$strain rate).

```
units           metal
echo            both
atom_style      atomic
dimension       3
boundary        s p s
region          box block 0 50 0 100 0 50  units box
create_box      3 box

lattice         fcc 4.05
region          Al block 0 50 0 100  0 50 units box
create_atoms    1 region Al units box
group           matrix region Al

region          2 sphere 4 4 4 4 units box
delete_atoms    region 2
region          3 sphere 46 46 46 4 units box
```

```
delete_atoms      region 3
region            4 sphere 46 4 4 4 units box
delete_atoms      region 4
region            5 sphere 4 46 4 4 units box
delete_atoms      region 5
region            6 sphere 4 4 46 4 units box
delete_atoms      region 6
region            7 sphere 46 46 4 4 units box
delete_atoms      region 7
region            8 sphere 46 4 46 4 units box
delete_atoms      region 8
region            9 sphere 4 46 46 4 units box
delete_atoms      region 9
region            10 sphere 46 96 46 4 units box
delete_atoms      region 10
region            11 sphere 4 96 4 4 units box
delete_atoms      region 11

lattice           fcc 2.87
region            fe1 sphere 4 4 4 4 units box
create_atoms      2 region fe1 units box
group             clu1 region fe1

set               region fe1 type/fraction 3 0.25 12358
lattice           fcc 2.87
region            fe2 sphere 46 46 46 4 units box
create_atoms      2 region fe2 units box
group             clu2 region fe2

set               region fe2 type/fraction 3 0.25 12358
lattice           fcc 2.87
```

```
region          fe3 sphere 46 4 4 4 units box
create_atoms    2 region fe3 units box
group           clu3 region fe3

set             region fe3 type/fraction 3 0.25 12358
lattice         fcc 2.87
region          fe4 sphere 4 46 4 4 units box
create_atoms    2 region fe4 units box
group           clu4 region fe4

set             region fe4 type/fraction 3 0.25 12358
lattice         fcc 2.87
region          fe5 sphere 4 4 46 4 units box
create_atoms    2 region fe5 units box
group           clu5 region fe5

set             region fe5 type/fraction 3 0.25 12358
lattice         fcc 2.87
region          fe6 sphere 46 46 4 4 units box
create_atoms    2 region fe6 units box
group           clu6 region fe6

set             region fe6 type/fraction 3 0.25 12358
lattice         fcc 2.87
region          fe7 sphere 46 4 46 4 units box
create_atoms    2 region fe7 units box
group           clu7 region fe7

set             region fe7 type/fraction 3 0.25 12358
lattice         fcc 2.87
region          fe8 sphere 4 46 46 4 units box
```

```
create_atoms        2 region fe8 units box
group               clu8 region fe8

set                 region fe8 type/fraction 3 0.25 12358
lattice             fcc 2.87
region              fe9 sphere 46 96 46 4 units box
create_atoms        2 region fe9 units box
group               clu9 region fe9
set                 region fe9 type/fraction 3 0.25 12358

lattice             fcc 2.87
region              fe10 sphere 4 96 4 4 units box
create_atoms        2 region fe10 units box
group               clu10 region fe10
set                 region fe10 type/fraction 3 0.25 12358

timestep            0.002
pair_style          eam/fs
pair_coeff          * * AlFe_mm.eam.fs Al Fe Al

# Energy Minimization
minimize            1.0e-3 1.0e-6 10000 100000
compute             csym all centro/atom fcc
compute             peratom all pe/atom
variable            tmp equal ly
variable            lo equal ${tmp}
variable            strain equal (ly-v_lo)/v_lo
variable          p1 equal "-pxx/10000"
variable          p2 equal "-pyy/10000"
variable          p3 equal "-pzz/10000"
variable          p12 equal "-pxy/10000"
```

variable p23 equal "-pyz/10000"
variable p13 equal "-pxz/10000"

variable fm equal "(v_p2+v_p3+v_p1)/3" ##### Hydrostatic stress

variable fv equal "sqrt(((v_p2-v_p3)^2+(v_p3-v_p1)^2+(v_p1-v_p2)^2+6*(v_p12^2+v_p23^2+v_p13^2))/2)" ######Von Mises stress.

variable t equal "v_fm/v_fv"

variable fd equal (((v_p2-v_fm)*(v_p3-v_fm)*(v_p1-v_fm))-(v_p12)^2*(v_p3-v_fm)-(v_p13)^2*(v_p2-v_fm)-(v_p23)^2*(v_p1-v_fm)+2*v_p12*v_p23*v_p13)####Deviatoric Von Mises stress

# principal stresses

variable I1 equal "(v_p1+v_p2+v_p3)"

variable I2 equal "((v_p1)*(v_p2))+((v_p2)*(v_p3))+((v_p1)*(v_p3))-(v_p12)^2-(v_p23)^2-(v_p13)^2"

variable I3 equal "((v_p1)*(v_p2)*(v_p3))-((v_p1)*((v_p23)^2))-((v_p2)*((v_p13)^2))-((v_p3)*((v_p12)^2))+2*(v_p12)*(v_p23)*(v_p13)"

variable A equal "(acos(((2*(v_I1)^3)-9*(v_I1)*(v_I2)+27*(v_I3))/(2*((v_I1)^2-(3*(v_I2)))^(3/2))))/3"

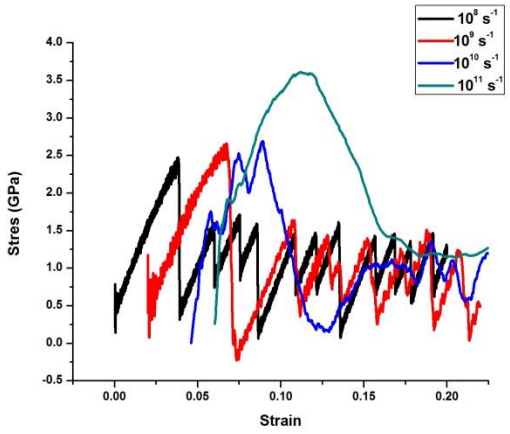
variable s1 equal "((v_I1)/3)+(2/3)*(sqrt((v_I1)^2-(3*(v_I2))))*cos(v_A)"

variable s2 equal "((v_I1)/3)+(2/3)*(sqrt((v_I1)^2-(3*(v_I2))))*cos((v_A)+(2*PI)/3)"

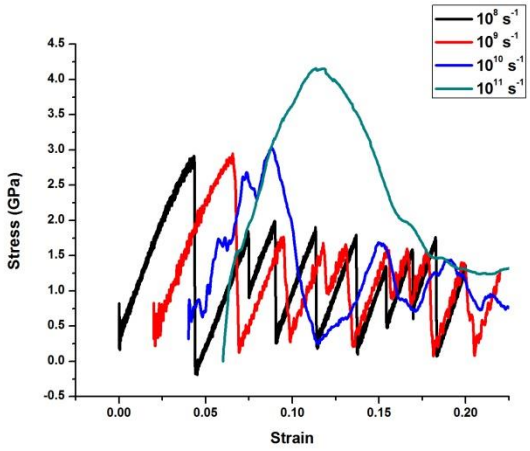
```
variable        s3 equal "((v_I1)/3)+(2/3)*(sqrt((v_I1)^2-(3*(v_I2))))*cos((v_A)+(4*PI)/3)"

thermo          100
thermo_style    custom step temp  vol press pe ke etotal
dump            1 all custom 100 compression_mmc.lammpstrj id type x  y z
dump            2 all cfg 100 dump.compress_mmc*.cfg id type xs ys zs c_csym c_peratom
dump            3 all custom 100 stress_peratom* id type xs ys zs c_1[1] c_1[2] c_1[3] c_1[4]
c_1[5] c_1[6]

log             NVTlog5050_compress_mmc.data
velocity        all create 300 873847 rot yes mom yes dist gaussian

# tensile deformation
 fix            2 all deform 1 y erate -0.01 units box
# temperature controller
fix             1 all nvt temp 300 300 0.01
fix             def all print 1 "${strain} ${p2} ${s1} ${s2} ${s3} ${fm} ${fv} ${t} ${fd}"
file mmc_compression_von.txt
run             10000
```

## 4.2.1 Effect of strain rate

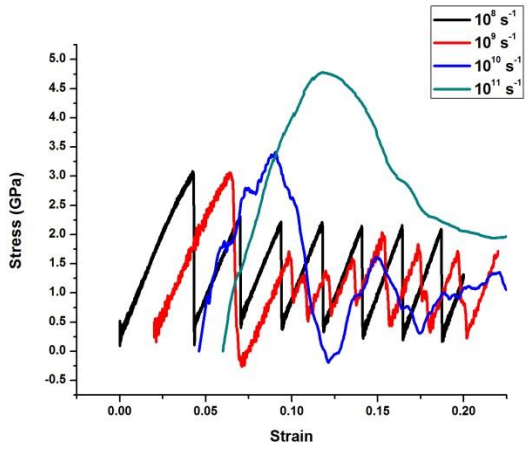
Fig.4.2 shows the various stress vs strain plots of Al metal matrix composite at different strain rates ($10^8$ $s^{-1}$ to $10^{11}$ $s^{-1}$) and at different temperatures (300K, 200K, 100K, 50K, and 10K). The strength of the material is increasing with the strain rate.



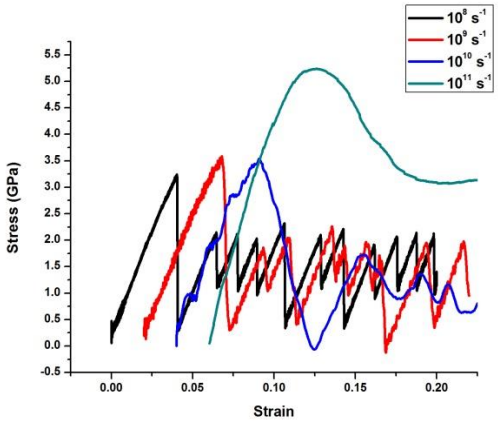

(a)



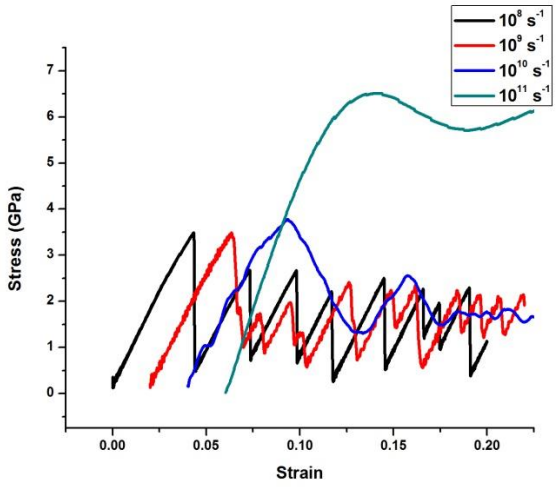

(b)




(c)




(d)

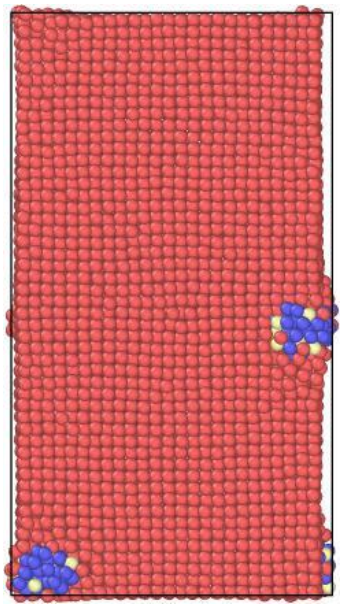



(e)

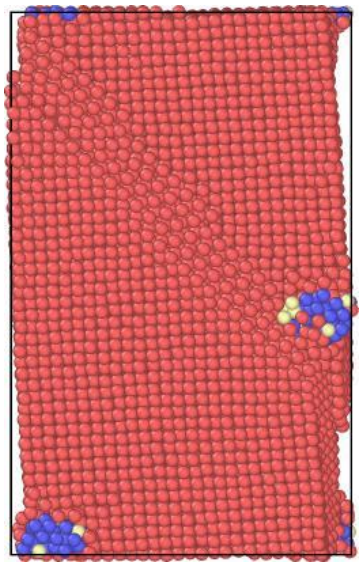
Fig.4.2 Shows the variation of strength of the model alloy with reinforcement volume at different temperatures (a) 300K (b) 200K (c) 100K (d) 50K (e) 10K.

## 4.2.2 Atomic position snap shots of Al MMC

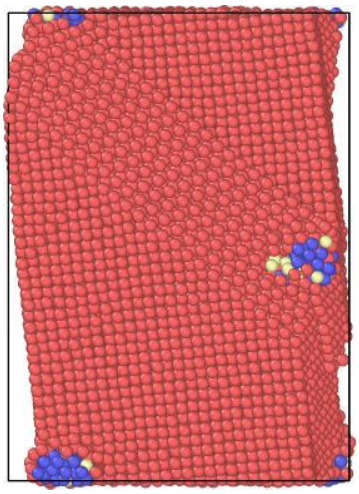
Ovito software is used to imagine the actions carried out in MD simulation. With the help of this software we can observe how the atoms are behaving and their positions at different strain conditions viz. 0%, 6%, 13% and 20% at $10^{10}$ $s^{-1}$ strain rate. From the below figures, we can detect that at 0% strain value, model alloy is in crystalline form, successively with increasing in strain value model alloy is deforming.



ε =0



ε =0.06



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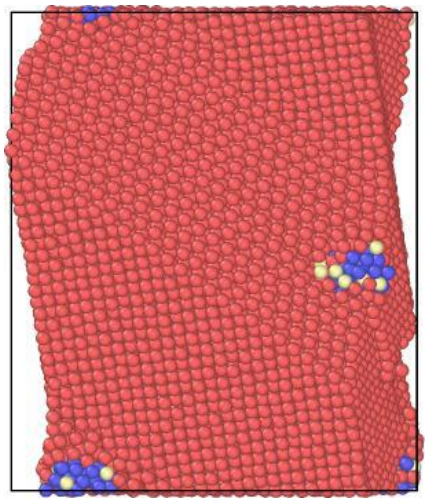

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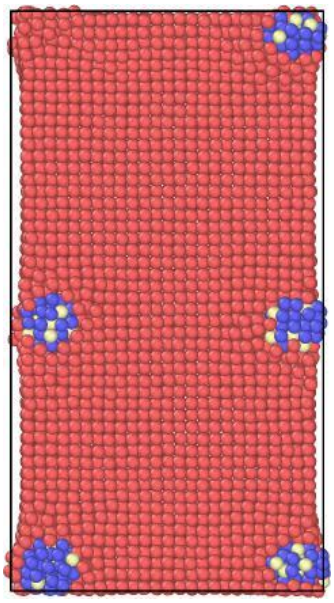
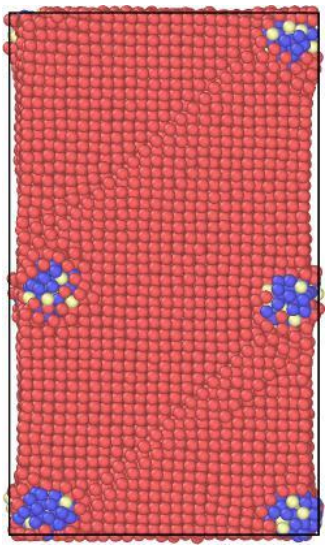
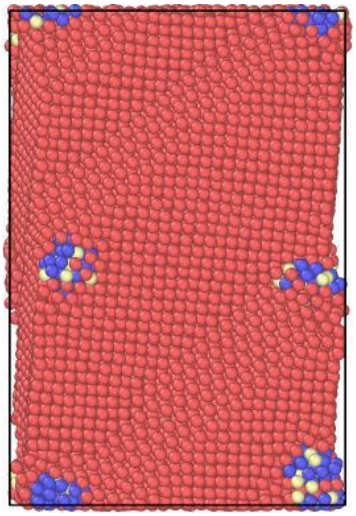
Fig.4.3 Snapshots showing the atomic arrangement in Al-5% $Fe_3Al$ MMC at different strain values at 300 K and at a strain rate of $10^{10}$ $s^{-1}$.



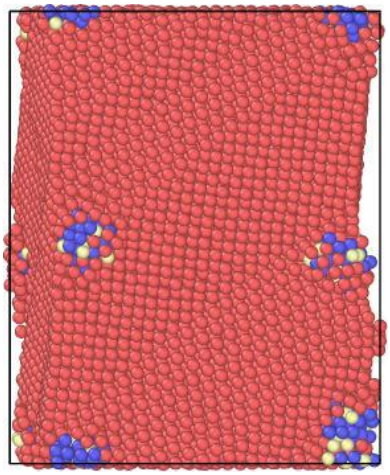
ε =0



ε =0.06

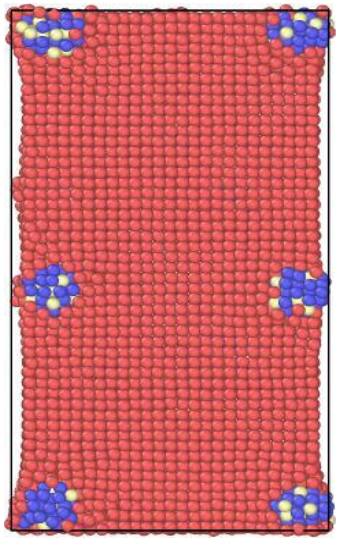


ε =0.13

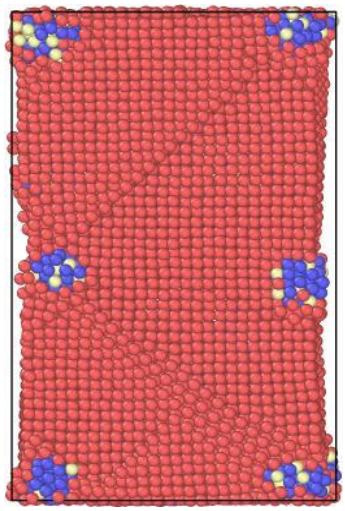


ε =0.2

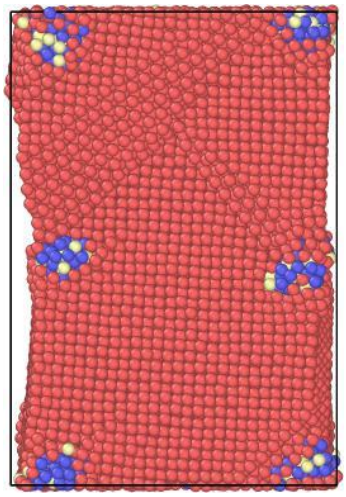
Fig.4.4 Snapshots showing the atomic arrangement in Al-10% $Fe_3Al$ MMC at different strain values at 300 K and at a strain rate of $10^{10}$ $s^{-1}$.



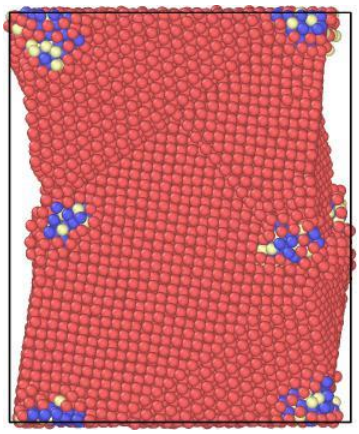
ε =0



ε =0.06

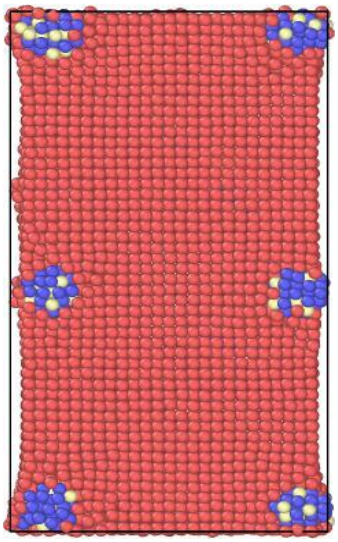


ε =0.13

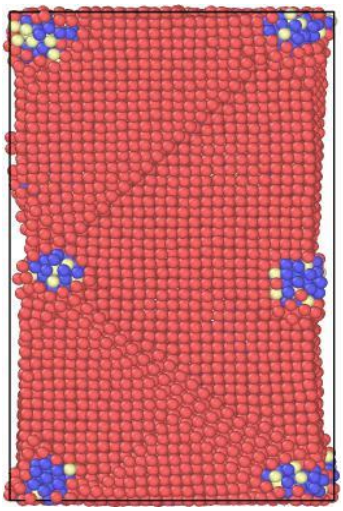


ε =0.2

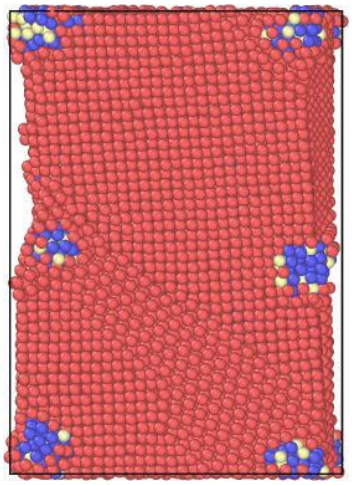
Fig.4.5 Snapshots showing the atomic arrangement in Al-15% $Fe_3Al$ MMC at different strain values at 300 K and at a strain rate of $10^{10}$ $s^{-1}$.



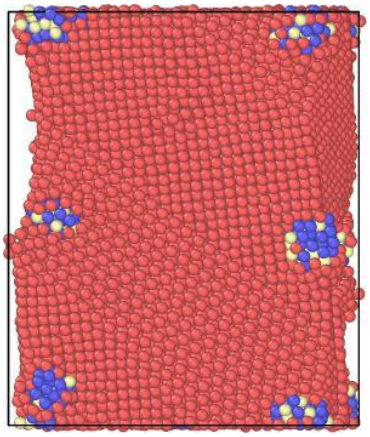
ε =0



ε =0.06

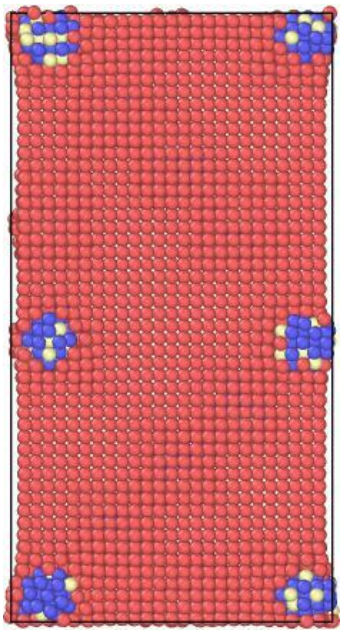


ε =0.13

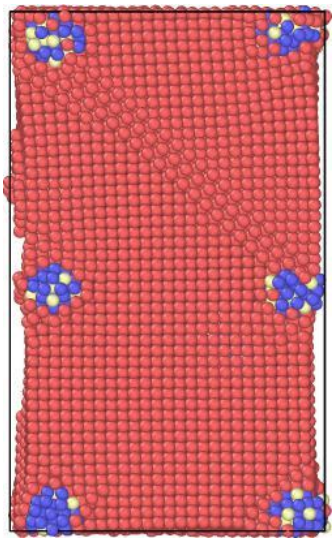


ε =0.2

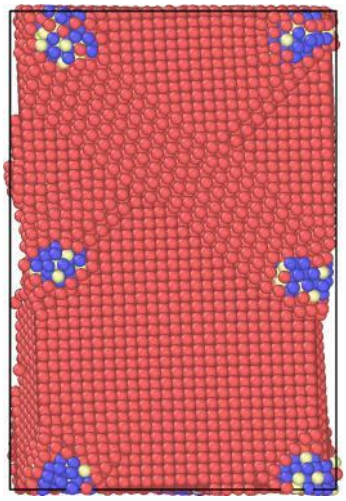
Fig.4.6 Snapshots showing the atomic arrangement in Al-20% $Fe_3Al$ MMC at different strain values at 300 K and at a strain rate of $10^{10}$ $s^{-1}$.



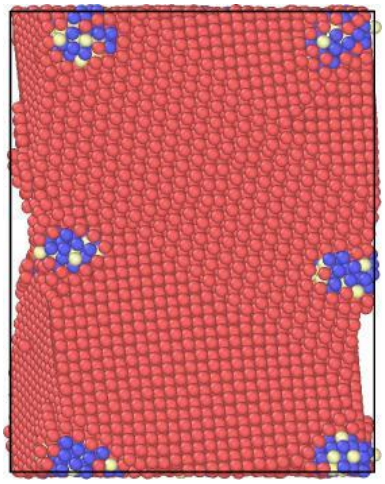
ε =0



ε =0.06



ε =0.13

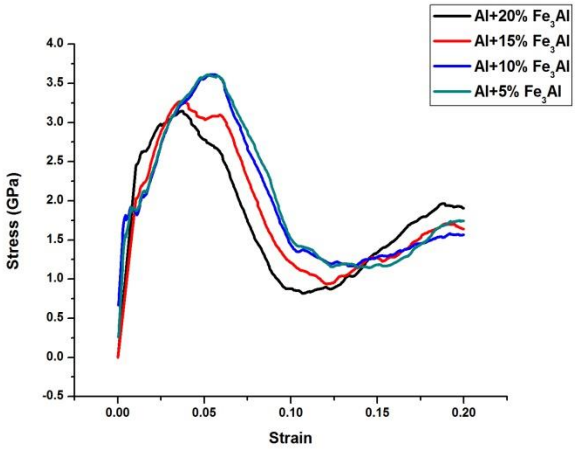


ε =0.2

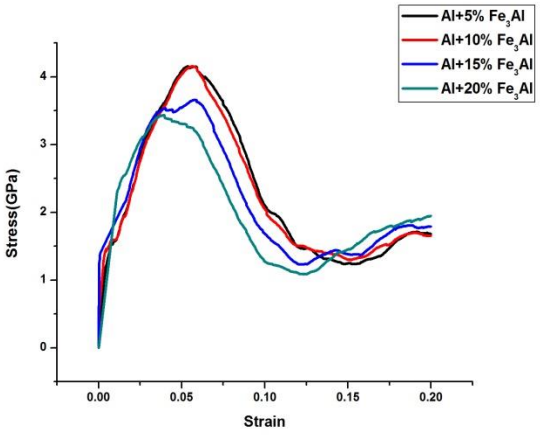
Fig.4.7 Snapshots showing the atomic arrangement in Al-20% $Fe_3Al$ MMC at different strain values at 10 K and at a strain rate of $10^{10}$ $s^{-1}$.

## 4.2.3 Effect of reinforcement volume fraction

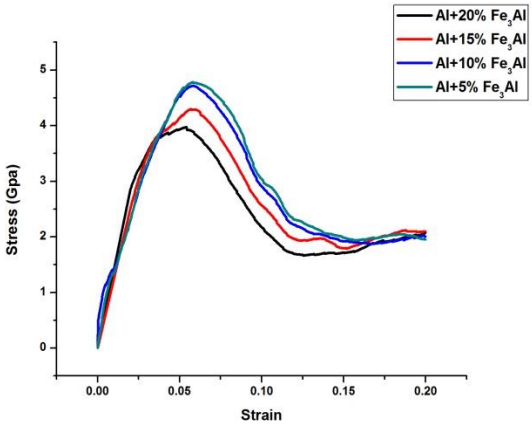
Fig.4.8 shows the various stress vs strain plots of Al MMC model reinforced with different volume fractions (5%, 10%, 15%, and 20%) at different temperatures viz. 300K, 200K, 100K, 50K, 10K. The strength of the composite is increasing with the reinforcement volume up to 10% vol. fraction.



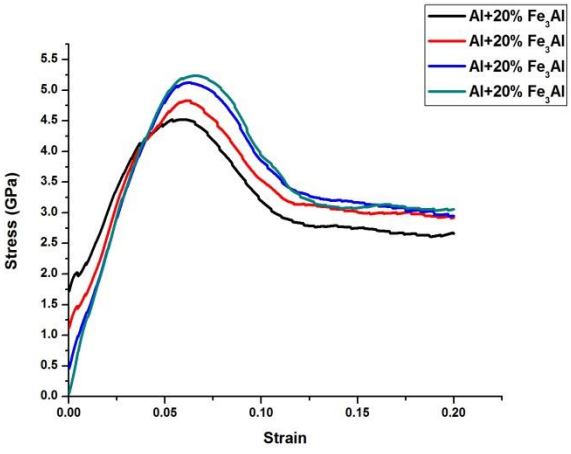

(a)



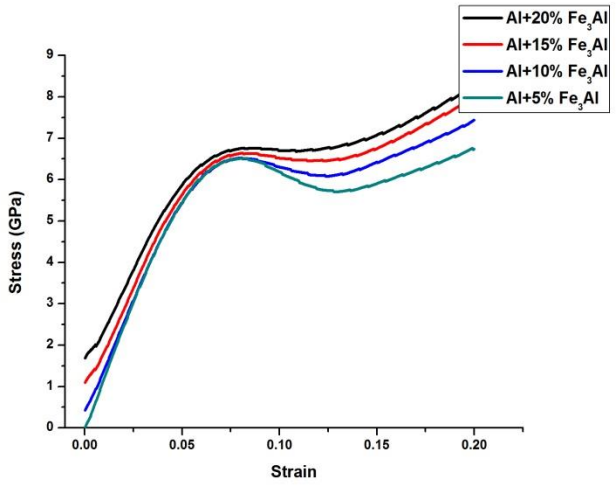

(b)




(c)




(d)

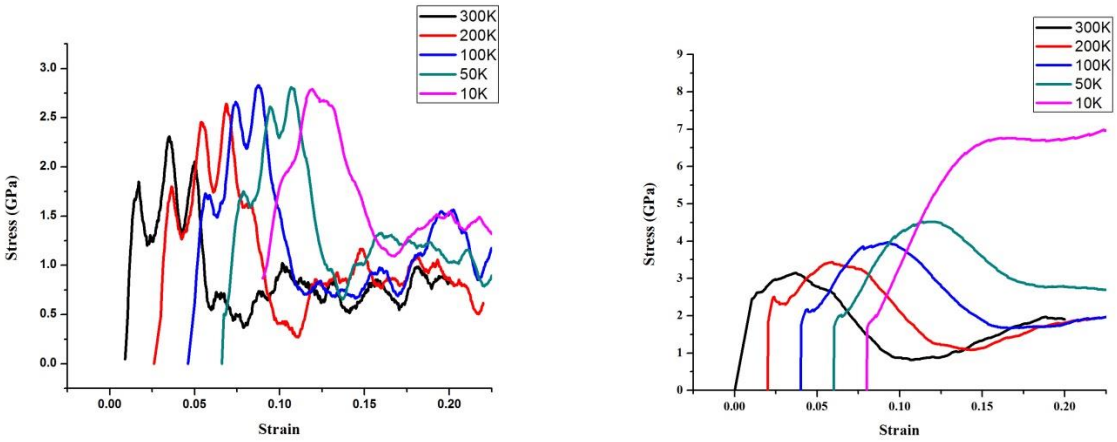



(e)

Fig.4.8 Shows the variation of strength of the model alloy with reinforcement volume at different temperatures (a) 300K (b) 200K (c) 100K (d) 50K (e) 10K.

## 4.2.4 Effect of Temperatures

Figure 4.9 shows the stress vs strain curves of Al metal matrix composite at different temperatures at viz. 300K, 200K, 100K, 50K, and 10K at two different strain rates ($10^{10}$ $s^{-1}$ and $10^{11}$ $s^{-1}$). It has been shown that with decreasing temperatures the value of stress increases.




(a) (b)

Fig.4.9 Shows variation of stress with temperatures (300K, 200K, 100K, 50K and 10K) of model alloy at two different strain rates (a) $10^{10}$ $s^{-1}$ (b) $10^{11}$ $s^{-1}$.

### 4.2.5 Young's modulus variation

From the simulation results the effect of reinforcement volume on the Young's modulus of Aluminium MMC at different temperatures, which are arranged in Table 4.1. From Table 4.1 we can observe that Young's modulus significantly varies w.r.t temperatures. The value of Young's modulus is decreasing with increasing the volume fraction of reinforcement. The effect of different volume fractions on Young's modulus of Al MMC depicted in Fig.4.10.

Table 4.1 Variation of Young's modulus as a function of reinforcement volume in Al MMC at different temperatures.

| MMC | Reinforcement volume (Volume %) | Young's Modulus (GPa) (300K) | Young's Modulus (GPa) (200K) | Young's Modulus (GPa) (100K) | Young's Modulus (GPa) (50K) | Young's Modulus (GPa) (10K) |
|---|---|---|---|---|---|---|
| Al-$Fe_3Al$ | 5 | 50.25 | 64.02 | 82.73 | 86.67 | 97.44 |
| | 10 | 46.18 | 60.79 | 76.92 | 82.67 | 91.44 |
| | 15 | 58.98 | 70.64 | 51.85 | 67.55 | 72.69 |
| | 20 | 32.5 | 52.70 | 40.64 | 60.19 | 69.21 |

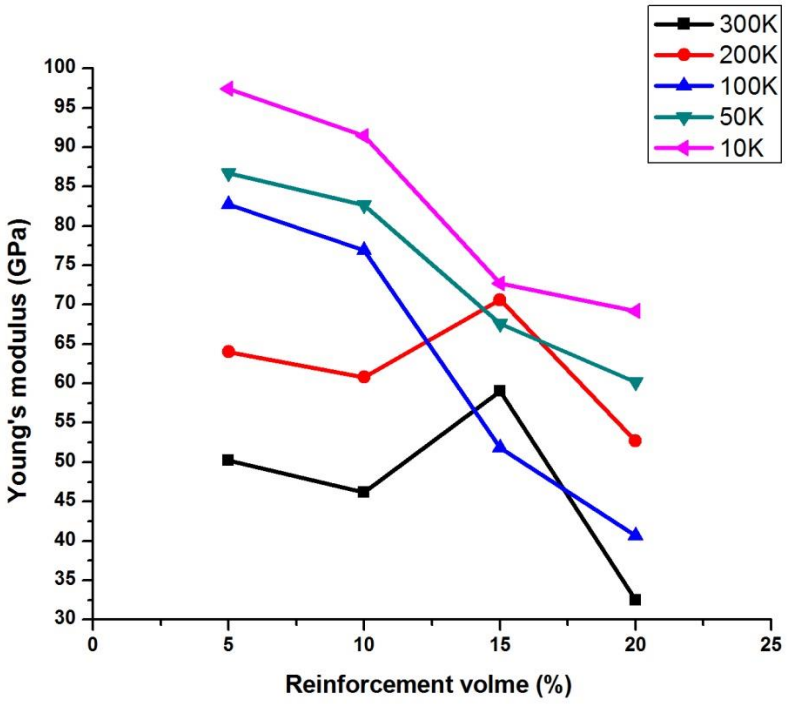



Fig.4.10 Young's modulus vs Reinforcement volume

## 4.2.6 Ultimate tensile Strength variation

From the simulation results the effect of reinforcement volume on the ultimate tensile strength of Aluminium MMC at different temperatures, which are arranged in Table 4.2. From Table 4.2 we can observe that ultimate tensile strength significantly varies w.r.t temperatures. The value of ultimate tensile strength is decreasing with increasing the volume fraction of reinforcement. The effect of different volume fractions on ultimate tensile strength of Al MMC depicted in Fig.4.11.

Table 4.2 Variation of ultimate tensile strength as a function of reinforcement volume in Al MMC at different temperatures.

| MMC | Reinforcement volume (Volume %) | Ultimate tensile Strength (GPa) (300K) | Ultimate tensile Strength (GPa) (200K) | Ultimate tensile Strength (GPa) (100K) | Ultimate tensile Strength (GPa) (50K) | Ultimate tensile Strength (GPa) (10K) |
|---|---|---|---|---|---|---|
| Al-$Fe_3Al$ | 5 | 3.575 | 4.14 | 4.73 | 5.23 | 6.45 |
| | 10 | 3.57 | 4.14 | 4.66 | 5.124 | 6.45 |
| | 15 | 3.24 | 3.65 | 4.27 | 4.81 | 6.59 |
| | 20 | 3.12 | 3.38 | 3.95 | 4.5 | 6.7 |

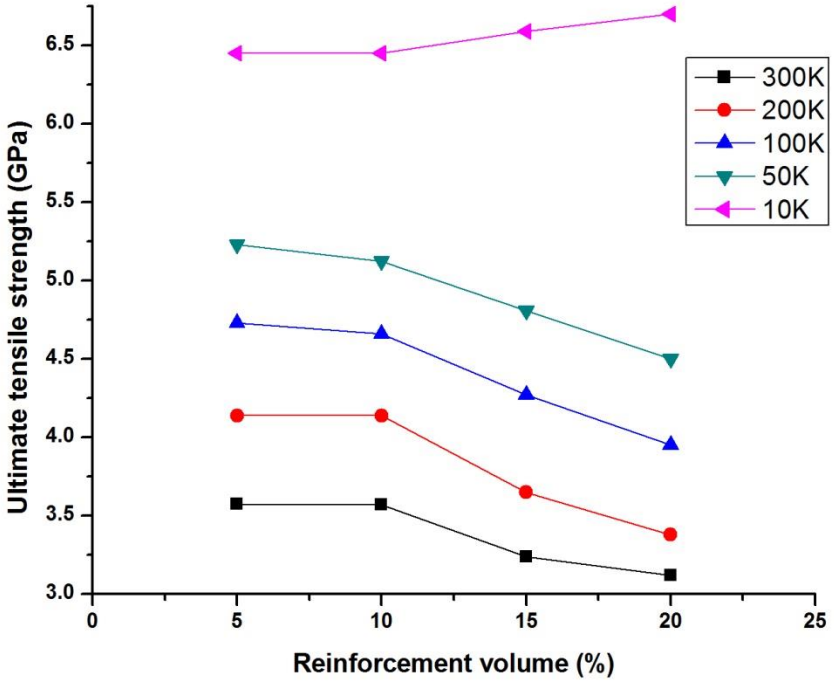



Fig.4.11 Ultimate tensile strength vs reinforcement volume

# CHAPTER 5

# 5. Conclusions

a) Experimental studies suggest that the strength of the material increases with the addition of $Fe_3Al$ as reinforcement.
b) MD simulations also show that addition of $Fe_3Al$ as reinforcement improves the strength of aluminum matrix.
c) MD simulations suggest that mechanical properties such as yield strength, ultimate strength increase with increase in volume fraction of the reinforcement (up to 10 vol.%)
d) MD compression studies at 10 K show an increase in yield strength even beyond 10 vol. % of Fe3Al. The reason for the above is due to increase in defect density.

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